The identity of the Hubbard Model upon cooling - Cluster dynamical mean-field and quantum Monte Carlo perspective

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Outline

Is the Hubbard model superconducting?

How does superconductivity arise in the presence of a pseudogap?
Cuprates and the Hubbard Model

Figure 1

T
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10.1038/NPHYS3009

from Barišić et al., Nat. Phys. 2013

from Hashimoto et al., Nat. Phys. 2014
Cuprates and the Hubbard Model

\[ H = \sum_{ij,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

Parameters:
- \( t \): nearest neighbor hopping
- \( t' \): next-nearest neighbor hopping
- \( U \): On-site Coulomb repulsion
Cuprates and the Hubbard Model

\[ \mathcal{H} = \sum_{ij,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

Parameters:
- \( t \): nearest neighbor hopping
- \( t' \): next-nearest neighbor hopping
- \( U \): On-site Coulomb repulsion

Single band near Fermi energy

![Image](image1.jpg)

from Hashimoto et al., Nat. Phys. 2014

from Barisic et al., Nat. Phys. 2013
Cuprates and the Hubbard Model

\[ \mathcal{H} = \sum_{ij,\sigma} t_{ij} c_{i\sigma}^+ c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

Parameters:
- \( t \): nearest neighbor hopping
- \( t' \): next-nearest neighbor hopping
- \( U \): On-site Coulomb repulsion

Does the Hubbard model have a superconducting state?
Pairing in the Hubbard model: Pre - Quantum Cluster Period

Pair-field susceptibility

\[
P_d = \int_0^\infty d\tau \left( \mathcal{T} \Delta_d(\tau) \Delta_d^\dagger(0) \right)
\]

\[
\Delta_d^\dagger = \sum_k (\cos k_x - \cos k_y) c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger
\]

DQMC on 4 x 4 Hubbard lattice with U=4t

White et al., PRB '89

1989
Pairing in the Hubbard model: Pre - Quantum Cluster Period

Pair-field susceptibility

\[ P_d = \int_0^\infty d\tau \langle \mathcal{F}_\tau \Delta_d(\tau)\Delta_d^\dagger(0) \rangle \]

\[ \Delta_d^\dagger = \sum_k (\cos k_x - \cos k_y) c_{k\uparrow}^\dagger c_{-k\downarrow} \]

DQMC on 4 x 4 Hubbard lattice with U=4
White et al., PRB '89

1989

DQMC on 8 x 8 Hubbard lattice with U=4
Bulut, Scalapino, White, PRB '93

1993

\[ d \text{-wave pair-field susceptibility} \]
Pairing in the Hubbard model: Pre - Quantum Cluster Period

**Diagram**: d-wave pair-field susceptibility

Pair-field susceptibility

\[ P_d = \int_0^\infty d\tau \langle \mathcal{T}_\tau \Delta_d(\tau)\Delta_d^+(0) \rangle \]

\[ \Delta_d^+ = \sum_k (\cos k_x - \cos k_y) c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger \]

**QMC sign problem** prevents calculations at sufficiently low temperatures

- **1989**: DQMC on 4 x 4 Hubbard lattice with U=4t
  - *White et al., PRB ’89*

- **1993**: DQMC on 8 x 8 Hubbard lattice with U=4t
  - *Bulut, Scalapino, White, PRB ’93*
Quantum Cluster Theories

Finite size approximations
(ED, DMRG, DQMC, …)

Dynamical mean field theory
Metzner & Vollhardt, PRL '89
Müller-Hartmann, Z. Phys. B '89
Georges et al., RMP '96
Quantum Cluster Theories

Finite size approximations
(ED, DMRG, DQMC, …)

Quantum cluster theories
(DCA, CDMFT, CPT, VCA, …)

Dynamical mean field theory
Metzner & Vollhardt, PRL ’89
Müller-Hartmann, Z. Phys. B ’89
Georges et al., RMP ’96

Hettler et al., PRB ’98
Liechtenstein & Katsnelson, PRB ’00
Kotliar et al., PRL ’01
TAM, Hettler, Pruschke & Jarrell, RMP ’05
Dynamical Cluster Approximation

Infinite size lattice

(1) Coarse-graining
\[ G(K,iω_n) = \frac{N}{N} \sum_{k \in \mathcal{K}} G(k,iω_n) = \frac{N}{N} \sum_{k \in \mathcal{K}} \frac{1}{iω_n - ε_k + Σ(K,iω_n)} \]

(2) Cluster exclusion
\[ c_f(K,iω_n) = \frac{1}{c(K,iω_n)} \]

(3) Quantum Monte Carlo cluster solver
\[ S[ϕ^*, φ] = -\int_0^β dt \int_0^β dt' \sum_{\eta} \bar{ϕ}_\eta^*(t) G_{i,j,k}(t-t') ϕ_\eta(t) + \int_0^β dt \sum_i U_\eta \bar{ϕ}_\eta(t) ϕ_\eta(t) \]
\[ G_{i,j,k}(t-t') = \frac{1}{Z} \int [\mathcal{D}[ϕ^*][ϕ] e^{-S[ϕ^*,φ]}] \]

(4) New self-energy
\[ Σ(K,iω_n) = G_0^{-1}(K,iω_n) - G_0^{-1}(K,iω_n) \]

DCA self-consistently maps infinite size lattice to effective cluster embedded in dynamic mean-field that describes the remaining lattice degrees of freedom

Cluster embedded in mean-field

Numerically exact solution of effective cluster problem with quantum Monte Carlo

Hettler, Tahvildar-Zadeh, Jarrell, Pruschke, Krishnamurthy, PRB '98
Maier, Jarrell, Pruschke, Hettler, RMP '05
Quantum cluster theory of superconductivity in the Hubbard model

Antiferromagnetism and d-wave superconductivity in cuprates: A cluster dynamical mean-field theory

Antiferromagnetism and d-wave superconductivity in the two-dimensional Hubbard model using a cluster DMFT scheme.

First quantum cluster calculations

d-Wave Superconductivity in the Hubbard Model

θ, M, θ, J. Keller, and M. I. Katsnelson

A microscopic theory of high-temperature superconductivity in cuprates [1]. Angle resolved photoemission experiments show evidence for a superconducting state with two different types of the order parameters: AFM and SC. In underdoped materials even in the normal state this pseudogap persists and the existence of a sharp 41 meV resonance [2]. In underdoped cuprates [1] the pseudogap as well as the transition to a superconducting phase, i.e., the physical origin of the pairing gap is an effective hopping and particle methods like the fluctuation exchange approximation ignores the vertex corrections in the strong correlation regime with Coulomb repulsion.

First quantum cluster calculations with two nonzero order parameters exist in a wide range of doping level and temperature [3,4]. We present an approach to investigate the interplay of antiferromagnetism and superconducting order parameter due to the presence of underlying antiferromagnetic ordering.

The minimal cluster which allows us to study both AFM and SC in the superconducting state. The near-net-doping regime with Coulomb repulsion is of low energy excitations.

Self-consistent solutions with two nonzero order parameters exist in a wide range of doping level and temperature. First quantum cluster calculations with two nonzero order parameters exist in a wide range of doping level and temperature. First quantum cluster calculations with two nonzero order parameters exist in a wide range of doping level and temperature.
Quantum cluster theory of superconductivity in the Hubbard model

Antiferromagnetism and \( d \)-wave superconductivity in cuprates: A cluster dynamical mean-field theory

A. I. Lichtenstein\(^1\) and M. I. Katsnelson\(^2\)

Phase diagram of the Hubbard model: Beyond the dynamical mean field

M. Jarrell\(^1\), Th. Maier\(^3\), M. H. Rettner\(^4\) and A. N. Tanisvili\(^5\)

\( d \)-Wave Superconductivity in the Hubbard Model

Th. Maier\(^3\), M. Jarrell\(^1\), Th. Pruschke\(^3\) and J. Kells\(^4\)
Quantum cluster theory of superconductivity in the Hubbard model
Quantum cluster theory of superconductivity in the Hubbard model
Quantum cluster theory of superconductivity in the Hubbard model
Larger U

\[ U = 4t, \langle n \rangle = 0.9 \]

\[ \lim_{N_c \to \infty} T_{KT}(N_c) = 0.0199 \pm 0.0019 \]

Consistent with Kosterlitz-Thouless scaling

\[ T_c(N_c) = T_{KT}^c + \frac{A}{B + \log(\sqrt{N_c})^2} \]

- Highest \( T_c \) for \( U \sim W = 8t \)

Staar et al., PRB '14
Larger U

\[ U = 4t, \langle n \rangle = 0.9 \]

\[ T_c \sim 0.05t \]

\[ U = 7t, \langle n \rangle = 0.9 \]

\[ T_c \sim 0.05t \]

\[ \lim_{N_c \to \infty} T_{KT}(N_c) = 0.0199 \pm 0.0019 \]

\[ T_c(N_c) = T_{cKT} + \frac{A}{[B + \log(\sqrt{N_c})]^2} \]

- Highest \( T_c \) for \( U \sim W=8t \)

Staar et al., PRB ’14
Stripes?

ARTICLE OPEN
Stripe order from the perspective of the Hubbard model

Edwin W. Huang, Christian B. Mendel, Hong-Chen Jiang, Brian Montz and Thomas P. Devereaux

DQMC on 16 x 4 Hubbard:
\[ U/t = 6, t'/t = -0.25, T/t = 0.22 \]
ARTICLE

Stripe order from the perspective of the Hubbard model

Edwin W. Huang1, Christian B. Mendel1, Hong-Chen Jiang1, Brian Mont2,∗ and Thomas P. Devereaux1,∗

CT-AUX on finite size 16 x 4 cluster
U/t = 5, t′/t = −0.25, T/t = 0.22

DQMC on 16 x 4 Hubbard:
U/t = 6, t′/t = −0.25, T/t = 0.22
CORRESPONDENCE: Thomas P. Devereaux (tpd@stanford.edu)
Materials, Stanford University, Stanford, CA 94305, USA

If the treatments are variational. On the other hand, provided that temperature properties requires rigorous effort to eliminate we use determinant quantum Monte Carlo (DQMC), an exact that shortened correlation lengths reduce temperatures.

Stripes order is nevertheless observable at accessible dimensions has led to development of various numerical diagonalization/dynamical mean-ties. Calculations to benchmark these techniques have revealed that different candidate ground states all lie close in energy, indicating striped ground states in the Hubbard model. A recent interplay of stripes with the aforementioned orders.

To understand these differences, we study the impact of neighbor hopping varying the model parameters, starting with the next-nearest-neighbor hopping. Figure displays the real space, equal-time spin correlation functions from DQMC at a temperature of $T/t = 0.25$, equivalent to 1/8 electron-doping for negative charge incommensurability, absent imposing inhomogeneity from artifacts of the anisotropic cluster geometry, we present and mensurate spin correlations. To ensure that these nuances and aspects of $\text{CT-AUX on finite size 16 x 4 cluster} \quad U/t = 5, t'/t = -0.25, T/t = 0.22$

$\text{DCA/CT-AUX (with mean-field)} \quad U/t = 5, t'/t = -0.25, T/t = 0.17$

$\text{DOMC on 16 x 4 Hubbard:} \quad U/t = 6, t'/t = -0.25, T/t = 0.22$
INTRODUCTION

The lack of an analytic solution to the Hubbard model in two-dimensions has led to development of various numerical methods to study its low temperature and ground state properties. Calculations. By varying temperature, doping, and model parameters, we characterize the extent of stripes throughout the phase diagram. Temperature calculations, from a variety of methods, have shown a variety of antiphase domain walls. Correlations functions for various hole doping levels. Dashed green lines indicate approximate locations of antiphase domain walls. Correlations functions (lower portion of Fig. 1) and pseudogap physics, interplay of stripes with the aforementioned orders.

The fermion sign problem sets a lower bound on the range of auxiliary temperatures. While calculations utilizing small clusters, of temperature technique, for this purpose. Although the worsening sign problem constrains the lowest accessible temperature calculations. In contrast, the period ~5 stripes from simulations and pseudogap physics, finding period-8 striped superconductivity in the Hubbard model, a minimal model believed to be relevant to the cuprate superconductors, using determinant field theory, constrained path symmetry breaking that is present across all cuprate families, commonly in the form of stripes. Here we investigate emergence of stripes in the ground state of the 1/8-hole-doped Hubbard model, providing evidence for period-8 stripes, and antiphase domain walls still evident from the checkerboard pattern, or equivalently the worsened sign problem constrains the lowest accessible temperature calculations. For half-filling (Fig. 1b), antiferromagnetic spin correlations are evident from the checkerboard pattern, or equivalently the worsted sign problem constrains the lowest accessible temperature calculations.

In our data, reduced correlation lengths at higher doping (Fig. 1a), antiferromagnetic spin correlations are evident from the checkerboard pattern, or equivalently the worsened sign problem constrains the lowest accessible temperature calculations. For half-filling (Fig. 1b), antiferromagnetic spin correlations are evident from the checkerboard pattern, or equivalently the worsened sign problem constrains the lowest accessible temperature calculations.

Variations in the interaction strength role of the value of $U/t$, $J/t$ and $\pi t/2$ for the lowest temperature accessible to simulation. For $t'/t = -0.25$, equivalent to 1/8 electron-doping for negative $U$, $\pi t/2 = 0.25$, as shown by our DMRG simulations in Fig. S2 of the Supplementary Materials. Spin correlations for $p = 0.042$ and $0.17$ of temperature to make little direct impact on electron-doped compounds similarly.

Other Parameters:

\[ U/t = 5, t'/t = -0.25, T/t = 0.22 \]

CT-AUX on finite size 16 x 4 cluster

DCA/CT-AUX (with mean-field)

\[ U/t = 5, t'/t = -0.25, T/t = 0.17 \]

- Mean-field coupling frustrates stripe formation and favors superconductivity

Stripe order from the perspective of the Hubbard model

Absence of an analytic solution to the Hubbard model in two-dimensions has led to development of various numerical methods to study its low temperature and ground state properties. Correlations functions for various hole doping levels. Dashed green lines indicate approximate locations of antiphase domain walls. Correlations functions (lower portion of Fig. 1) and pseudogap physics, interplay of stripes with the aforementioned orders.
**Pairing interaction and Bethe-Salpeter equation**

**Particle-particle Bethe-Salpeter equation** relates gap function $\phi(k)$ to pairing interaction $\Gamma(k, k')$

$$-\frac{T}{N} \sum_{k'} \Gamma(k, k') G(k') G(-k') \phi_{\alpha}(k') = \lambda_{\alpha} \phi_{\alpha}(k)$$

**BCS:**

$$-\frac{1}{N} \sum_{k'} V_{kk'} \Delta_{k'} \tanh \left( \frac{1}{2} \beta E_{k'} \right) \frac{\Delta_{k'}}{2E_{k'}} = \Delta_k$$
**Pairing interaction and Bethe-Salpeter equation**

**Particle-particle Bethe-Salpeter equation** relates gap function $\phi(k)$ to pairing interaction $\Gamma(k, k')$

$$\Gamma(k, k') \phi_{\alpha}(k') = \lambda_{\alpha} \phi_{\alpha}(k)$$

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**BCS:**

$$\frac{1}{N} \sum_{k'} V_{kk'} \Delta_{k'} \tanh\left(\frac{1}{2} \beta E_{k'}\right) = \Delta_k$$

**d-wave pair-field susceptibility**

$$P_d = \int_0^\beta d\tau \langle \mathcal{T} \Delta(\tau) \Delta^\dagger(0) \rangle$$

$$\Delta^\dagger = \frac{1}{\sqrt{N}} \sum_k g_d(k) c_{k_1^+}^\dagger c_{-k_1}^\dagger$$

$$P_d(T) \sim \frac{1}{1 - \lambda_d(T)}$$
Pairing interaction and Bethe-Salpeter equation

**Particle-particle Bethe-Salpeter equation** relates gap function \( \phi(k) \) to pairing interaction \( \Gamma(k, k') \)

\[
-\frac{T}{N} \sum_{k'} \Gamma(k, k')G(k')G(-k')\phi_d(k') = \lambda\phi_d(k)
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**BCS:**

\[
-\frac{1}{N} \sum_k V_{kk'} \Delta \tanh(\frac{1}{2}\beta E_{k'}) = \Delta_k
\]

**d-wave pair-field susceptibility**

\[
P_d(T) = \int_0^\beta d\tau \langle \mathcal{F}_\tau \Delta(\tau)\Delta^\dagger(0) \rangle
\]

\[
\Delta^\dagger = \frac{1}{\sqrt{N}} \sum_k g_d(k)c_{k1}^\dagger c_{-k1}^\dagger
\]

Separable approximation

\[
\lambda_d(T) \approx V_d(T)P_{d,0}(T)
\]

\[
V_d = -\langle \phi_d | \Gamma | \phi_d \rangle \; ; \; P_{d,0}(T) = \frac{T}{N} \langle \phi_d | GG | \phi_d \rangle
\]

**BCS:** \( V_d(T) \approx \text{const} \) ; \( P_{d,0}(T) \sim \log(t/T) \)
Structure of the pairing interaction

Momentum dependence

Frequency dependence

TAM et al., PRL ’06, PRB ’06
Structure of the pairing interaction

Pairing interaction carries spin $S=1$, increases with momentum transfer, and its dynamics reflects the spin fluctuation spectrum.

- Pairing interaction carries spin $S=1$, increases with momentum transfer, and its dynamics reflects the spin fluctuation spectrum.
Structure of the pairing interaction

Momentum dependence

Frequency dependence

- Pairing interaction carries spin S=1, increases with momentum transfer, and its dynamics reflects the spin fluctuation spectrum

TAM et al., PRL ‘06, PRB ‘06

PHYSICAL REVIEW B 80, 205109 (2009)

Pairing dynamics in strongly correlated superconductivity

B. Kyung, D. Sénchal, and A.-M. S. Tremblay
we start from the far-right side of Figure 1, in the overdoped metallic state. This state is characterized by a large Fermi surface that has a volume containing $1 + p$ holes per Cu atom, as determined by angle-dependent magneto-resistance (11), angle-resolved photoemission spectroscopy (12), and quantum oscillations (13), all performed on the single-layer cuprate Tl$_2$Ba$_2$CuO$_6$+$\delta$ (Tl-2201). The low-temperature Hall coefficient $R_H$ of overdoped Tl-2201 is positive and equal to $1 / e (1 + p)$ (14), as expected for a single-band metal with a hole density $n = 1 + p$. Conduction in the normal state obeys the Wiedemann-Franz law (15), a hallmark of Fermi-liquid theory. At the highest doping, beyond the superconducting phase (Figure 1), the electrical resistivity $\rho(T)$ of Tl-2201 exhibits the standard $T^2$ temperature dependence of a Fermi liquid (16), also observed in La$_{2-x}$Sr$_x$CuO$_4$ (LSCO) (17).

### 3. SCATTERING AND PAIRING

The question then is this: What makes superconductivity emerge from this particular, rather conventional, metal? The critical doping at which superconductivity springs is roughly the same in all hole-doped cuprates, namely $p_c$. Note that although it appears to obey weak-coupling BCS theory, at least initially (15, 18), the superconducting state has $d$-wave symmetry (19) rather than the usual $s$-wave symmetry, pointing to an electronic rather than phononic pairing mechanism (20). What happens at $p_c$ to make $d$-wave pairing prevail? Let us investigate one intriguing clue: At this special doping, the scattering between electrons undergoes a qualitative change. Indeed, it is precisely below $p_c$ that the pseudogap phase sets in below a crossover temperature $T_\text{c*}$, which goes to zero at a quantum critical point (QCP) located at $p_c$ in the absence of superconductivity (removed, for example, by application of a large magnetic field). The existence, nature, and location of such a QCP are a major focus of this review. In the presence of superconductivity, the QCP may move to lower doping, down to $p_S$, as a result of a competition between the pseudogap and superconducting phases (9, 10).
Superconductivity appears (below a critical temperature $T_\text{c}$) in a metal with a hole density $p$ that deviates from its Fermi-liquid behavior, acquiring a linear temperature dependence. The simultaneous onset of a pseudogap phase at a quantum critical point (QCP) located at $T_\text{N}$ is observed in the overdoped Tl-2201 cuprate. The metallic state shows all the signs of a conventional Fermi liquid. At the critical doping $p_c$, which vanishes rapidly with doping, the electrical resistivity $\rho(T)$ goes to zero at a QCP located at $T_\text{c}$ and $T_\text{N}$.

Superconductivity emerges at this special doping, as a result of a competition between the pseudogap and superconducting phases. Let us examine one intriguing clue: At this doping, the electronic rather than phononic pairing mechanism is observed. What happens at this state has not been fully understood, as it appears to obey weak-coupling BCS theory, at least initially.

The question then is this: What makes superconductivity emerge from this particular, rather conventional, metal? The critical doping at which superconductivity springs is $p_c$, as determined by angle-dependent magneto-resistance. In the presence of superconductivity, the QCP may move to lower temperatures below a crossover temperature $T_\text{c}$. In the absence of superconductivity, down to $p_s$, two events happen simultaneously: Superconductivity appears below a critical temperature $T_\text{c}$ and linear resistivity is the starting point for our exploration of cuprates. The evolution from metal to insulator is interrupted by the onset of the pseudogap phase that sets in below a crossover temperature $T_\text{c}$.

The hole density $x$ is proportional to the carrier density; when the Fermi level $E_F$ separates occupied states from unoccupied states, its volume is directly proportional to the number of occupied states. For materials with a single Fermi level, the Fermi-liquid strength $\alpha$ is proportional to the volume of their Fermi surface. The Fermi-liquid strength $\alpha$ is characterized by the volume containing $1 / 2$ of the Fermi level $E_F$.

In the overdoped Tl-2201 cuprate, the Fermi surface is characterized by a large Fermi surface that has a volume containing $1 / 2$ of the Fermi level. The Fermi-liquid strength $\alpha$ is characterized by the volume containing $1 / 2$ of the Fermi level.

The electric susceptibility $\chi$ results from the cyclotron motion and Landau quantization of energy levels; their frequency is proportional to the cross-sectional area $A$ of a closed Fermi surface. The bulk magnetic susceptibility $\chi(B)$ is proportional to the electric susceptibility $\chi$ and the cross-sectional area $A$ of the Fermi surface.

Quantum oscillations in the resistance or magnetization of a metal as a function of a magnetic field $B$ give information about the Fermi surface: hole-like (enclosing occupied states) or electron-like (enclosing unoccupied states); its volume is directly proportional to the number of occupied states. The Fermi-liquid strength $\alpha$ is characterized by the volume containing $1 / 2$ of the Fermi level.

The temperature dependence of a Fermi liquid, also observed in La$_{2-x}$Sr$_x$CuO$_4$ (LSCO) and other hole-doped cuprates, namely Tl-2201, is positive and equal to $1 / 2$ of $T_\text{c}$. This is the Franz law (15), a hallmark of Fermi-liquid theory.

The scattering between electrons undergoes a qualitative change below $T_\text{c}$ and linear resistivity is the starting point for our exploration of cuprates. The evolution from metal to insulator is interrupted by the onset of the pseudogap phase that sets in below a crossover temperature $T_\text{c}$.
we start from the far-right side of Figure 1, in the overdoped metallic state. This state is characterized by a large Fermi surface that has a volume containing 1\(+p\) holes per Cu atom, as determined by angle-dependent magneto-resistance (11), angle-resolved photoemission spectroscopy (12), and quantum oscillations (13), all performed on the single-layer cuprate \(\text{Tl}_2\text{Ba}_2\text{CuO}_6^{+d}(\text{Tl}-2201)\). The low-temperature Hall coefficient \(R_H\) of overdoped Tl-2201 is positive and equal to \(1/e(1+p)\) (14), as expected for a single-band metal with a hole density \(n=1+p\). Conduction in the normal state obeys the Wiedemann-Franz law (15), a hallmark of Fermi-liquid theory. At the highest doping, beyond the superconducting phase (Figure 1), the electrical resistivity \(\rho(T)\) of Tl-2201 exhibits the standard \(T^2\) temperature dependence of a Fermi liquid (16), also observed in La\(_{2-x}\)Sr\(_x\)CuO\(_4\) (LSCO) (17).

3. SCATTERING AND PAIRING

The question then is this: What makes superconductivity emerge from this particular, rather conventional, metal? The critical doping at which superconductivity springs is roughly the same in all hole-doped cuprates, namely \(p_c/\sqrt{2}\approx0.27\). Note that although it appears to obey weak-coupling BCS theory, at least initially (15, 18), the superconducting state has \(d\)-wave symmetry (19) rather than the usual \(s\)-wave symmetry, pointing to an electronic rather than phononic pairing mechanism (20). What happens at \(p_c\) to make \(d\)-wave pairing prevail? Let us investigate one intriguing clue: At this special doping, the scattering between electrons undergoes a qualitative change. Indeed, it is precisely below \(p_c\) that the pseudogap phase, which sets in below a crossover temperature \(T^*\), vanishes. The existence, nature, and location of such a QCP are a major focus of this review. In the presence of superconductivity, the QCP may move to lower doping, down to \(p_S\), as a result of a competition between the pseudogap and superconducting phases (9, 10).
Pseudogap in the 2D Hubbard Model

PHYSICAL REVIEW B 73, 165114 (2006)

Pseudogap induced by short-range spin correlations in a doped Mott insulator

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(Received 27 January 2006; revised manuscript received 21 February 2006; published 13 April 2006)

Valence bond dynamical mean-field theory of doped Mott insulators with nodal/antinodal differentiation

M. Ferrero¹, P. S. Corboz¹,4, L. De Leo¹, O. Parcollet², G. Kotliar³, and A. Georges⁴

PHYSICAL REVIEW B 82, 155101 (2010)

Momentum-space anisotropy and pseudogap: A comparative cluster dynamical mean-field analysis of the doping-driven metal-insulator transition in the two-dimensional Hubbard model

E. Gall¹, M. Ferrero², O. Parcollet³, A. Georges⁴, and A. J. Millis¹
Pairing in a dry Fermi sea

Normal metal: Cooper log instability

\[ P(T) \sim \frac{1}{1 - \lambda(T)} \]

\[ \lambda(T) = VP_0(T) \]

\[ P_0(T) \sim \log(a/T) \]

- Pairing interaction V is set at high T and SC instability arises from Cooper log divergence of pair propagator \( P_0(T) \)
Pairing in a dry Fermi sea

Normal metal: Cooper log instability

\[ P(T) \sim \frac{1}{1 - \lambda(T)} \]
\[ \lambda(T) = VP_0(T) \]
\[ P_0(T) \sim \log(a/T) \]

- Pairing interaction V is set at high T and SC instability arises from Cooper log divergence of pair propagator P_0(T)

\[ \text{Cuprate pseudogap phase: Absence of Cooper log divergence} \]

- Cooper log instability is absent and P_{d,0}(T) decreases for T < T^*

TAM et al., Nat. Comm. ‘16
In the pseudogap regime, it is the pairing interaction $V_d(T)$ that increases when $T$ decreases.

$$\lambda_d(T) \approx P_{0,d}(T)V_d(T)$$

TAM et al., Nat. Comm. ‘16
Spin-fluctuation interaction

Spin-fluctuation strength increases similar to the d-wave pairing kernel as $T$ is lowered.

Interaction
- irr. particle-particle vertex
- RPA spin-fluctuation interaction

\[
\phi^{PP}(k,\omega|k',\omega') \approx \frac{3}{2} U^2 \chi_S(k-k',\omega-\omega')
\]

$\lambda_d$ vs. $T$

"exact" eigenvalue

Eigenvalue from spin-fluctuation interaction

TAM et al., Nat. Comm. '16
Spin-fluctuation interaction

\[ \chi_{\text{RPA}}(q, \omega_m) = \frac{\chi_0(q, \omega_m)}{1 - \bar{U}\chi_0(q, \omega_m)} \]

\[ \chi_0(q, \omega_m) = -\frac{T}{N} \sum_{k,\omega_n} G(k + q, \omega_n + \omega_m)G(k, \omega_n) \]

From ARPES data on Bi2212 (\(T_c\sim 90\) K)

**Discussion**

The data that support the findings of this study are available on [this link](#).

The spin-fluctuation-mediated pairing interaction in a high-temperature superconductor.

**Methods**

The number of sites in the cluster. For the 4\(\times 4\) lattice, one would see the strength of the spin fluctuations found in the DCA calculation is at odds with the dynamic mean-field cluster is such that charge density and of the irreducible pairing interaction. In these calculations, the spin–fluctuation interaction provides a reasonable approximation for the d-wave pairing kernel as \(T\) is lowered.

**Figure 1**

- **d-wave eigenvalue (Hubbard model)**
  - Interaction
    - Irr. particle–particle vertex
    - RPA spin-fluctuation interaction
  - \(\zeta^{\text{pp}}(k, \omega|k', \omega') \approx \frac{3}{2} \hat{U}^2 \chi_{\text{S}}(k - k', \omega - \omega')\)

- **Spin-fluctuation strength increases similar to the d-wave pairing kernel as \(T\) is lowered**

**Equations**

- **Equation 1**
  \[ \chi_0(q, \omega_m) = -\frac{T}{N} \sum_{k,\omega_n} G(k + q, \omega_n + \omega_m)G(k, \omega_n) \]

- **Equation 2**
  \[ \chi_{\text{RPA}}(q, \omega_m) = \frac{\chi_0(q, \omega_m)}{1 - \bar{U}\chi_0(q, \omega_m)} \]

**Arrow Diagram**

- **Arrow 1**
  - **From ARPES data on Bi2212 (\(T_c\sim 90\) K)**

**Diagram**

- **Diagram 1**
  - **Graph**
    - X-axis: \(T\)
    - Y-axis: \(\lambda_d\)
    - Points: Black dots, magenta squares, pink squares
  - **Equation**
    - \(\zeta^{\text{pp}}(k, \omega|k', \omega') \approx \frac{3}{2} \hat{U}^2 \chi_{\text{S}}(k - k', \omega - \omega')\)

**Figure 2**

- **Graph**
  - X-axis: \(\omega_m/t\)
  - Y-axis: \(\lambda_d(\omega_m)\)
  - Points: Black dots, magenta squares, pink squares, cyan diamonds

**Text**

- **Text 1**
  - Spin-fluctuation strength increases similar to the d-wave pairing kernel as \(T\) is lowered

**Notes**

4. Nishiyama, S., Miyake, K. & Varma, C. M. Superconducting transition order 50 meV. Using a value of the coupling constant, the d-wave pairing kernel as \(T\) is lowered.
5. Gull, E., Parcollet, O. & Millis, A. J. Superconductivity and the pseudogap in the Hubbard model.
Nature of pair-field fluctuations across the superconducting dome

- Figure 1: Schematic DCA phase diagram (12-site cluster, U=7t, t'/t=-0.15)

Schematic phase diagram of cuprate superconductors as a function of hole doping.
Nature of pair-field fluctuations across the superconducting dome


Schematic DCA phase diagram
(12-site cluster, U=7t, t'/t=-0.15)

Doping dependence of $\varepsilon(T) = 1 - \lambda_d(T)$

$$P_d(T) = \frac{P_{d,0}(T)}{1 - \lambda_d(T)}$$

Bulk magnetic susceptibility $\chi_{\text{B}}(q=0,T)$

$\langle n \rangle = 0.850$

$\varepsilon(T) = 1 - \lambda_d(T)$

$\langle n \rangle = 0.85$
Doping dependence of $\varepsilon(T)$

Bulk magnetic susceptibility

Overdoped region

$$\varepsilon(T) = 1 - \lambda_d(T)$$

$$P_d(T) = \frac{P_{d,0}(T)}{1 - \lambda_d(T)}$$

$\langle n \rangle = 0.85$

$\varepsilon(T) \sim \ln(T/T_c)$

$P_d(T)$ is the doping-dependent susceptibility, with $P_{d,0}(T)$ representing the susceptibility at zero doping. The overdoped region is characterized by

$$\varepsilon(T) \sim \ln(T/T_c^{MF})$$

where $T_c^{MF}$ is the mean-field transition temperature.

TAM & Scalapino, npj Quant. Mat. ’19
Doping dependence of $\varepsilon(T)$

Bulk magnetic susceptibility

$$\chi_b(q=0,T) = 1 - \lambda_d(T)$$

Overdoped region

$$\varepsilon(T) \sim \ln(T/T_c^{MF})$$

$$P_d(T) = \frac{P_{d,0}(T)}{1 - \lambda_d(T)}$$
Doping dependence of $\varepsilon(T)$

\[
P_d(T) = \frac{P_{d,0}(T)}{1 - \lambda_d(T)}
\]

Overdoped region

$\varepsilon(T) \sim \ln(T/T_c^{MF})$
Doping dependence of $\varepsilon(T)$

\[ P_d(T) = \frac{P_{d,0}(T)}{1 - \lambda_d(T)} \]

Bulk magnetic susceptibility

\[ \langle n \rangle = 0.850 \]
\[ \langle n \rangle = 0.875 \]
\[ \langle n \rangle = 0.900 \]
\[ \langle n \rangle = 0.930 \]

⇒ Pseudogap in underdoped region

Overdoped region

\[ \varepsilon(T) \sim \ln(T/T_c^{MF}) \]

TAM & Scalapino, npj Quant. Mat. '19
Doping dependence of $\varepsilon(T)$

**Bulk magnetic susceptibility**

$P_d(T) = \frac{P_{d,0}(T)}{1 - \lambda_d(T)}$

$\varepsilon(T) = 1 - \lambda_d(T)$

**Overdoped region**

$\varepsilon(T) \sim \ln(T/T_c^{MF})$

**Underdoped region**

$\varepsilon(T) \sim T - \frac{\pi}{2}T_{KT}$

$\varepsilon(T) \sim e^{-\frac{B}{\sqrt{|T-T_{KT}|}}}$

⇒ Pseudogap in underdoped region

TAM & Scalapino, npj Quant. Mat. ‘19
Phase fluctuations in underdoped pseudogap region

- Amplitude of local pair-field limited by opening of pseudogap
- Increase in pairfield susceptibility reflects increase in phase coherence
This can be measured!

Junction pair tunneling current

\[ \langle I(V) \rangle = c \Delta_d P''(\omega = 2eV) \]

Ginzburg-Landau (ladder) approximation

\[ P_d(\omega) \sim \frac{1}{\epsilon(T) - \frac{i\omega}{\Gamma_0}}; \quad \epsilon(T) = 1 - \lambda_d(T); \quad \Gamma_0 = 8T_c/\pi \]

\[ I(V) \sim P''(\omega = 2eV) \sim \frac{2eV}{\Gamma_0} \frac{2eV}{\Gamma_0} \frac{2eV}{\Gamma_0} \frac{2eV}{\Gamma_0} \frac{2eV}{\Gamma_0} \frac{2eV}{\Gamma_0} \frac{2eV}{\Gamma_0} \frac{2eV}{\Gamma_0} \frac{2eV}{\Gamma_0} \frac{2eV}{\Gamma_0} \]

Generally

\[ P_d(\omega = 0,T) = \frac{P_{d,0}(T)}{1 - \lambda_d(T)} \sim \int dV I(V) / V \]

PAIR TUNNELING AS A PROBE OF FLUCTUATIONS IN SUPERCONDUCTORS

D. J. Scalapino
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(Received 10 March 1970)

Tunnel junction between S and S' with \( T_c(S) < T < T_c(S') \)

Scalapino, PRL 24, 1052 (1970)
This can be measured!

Junction pair tunneling current

\[ \langle I(V) \rangle = c\Delta_d P''(\omega = 2eV) \]

Ginzburg-Landau (ladder) approximation

\[ P_d(\omega) \sim \frac{1}{\epsilon(T) - i\omega \Gamma_0}; \epsilon(T) = 1 - \lambda_d(T); \Gamma_0 = 8T_c/\pi \]

\[ I(V) \sim P''(\omega = 2eV) \sim \frac{\frac{2eV}{\Gamma_0}}{\epsilon^2 + \left(\frac{2eV}{\Gamma_0}\right)^2} \]

Generally

\[ P_d(\omega = 0,T) = \frac{P_{d,0}(T)}{1 - \lambda_d(T)} \sim \int dV \frac{I(V)}{V} \]
Superconductivity in 2D Hubbard Model: Summary

- *Cluster dynamical mean field theory* finds robust *d-wave superconductivity in the doped 2D Hubbard model* (as well as a pseudogap)

- The *pairing interaction carries spin $S=1$*, increases with momentum transfer, and its dynamics reflects the *spin fluctuation* spectrum

- In the *overdoped region*, the superconducting instability arises from the conventional *Cooper log divergence* of the pair propagator

- In the *underdoped pseudogap region*, the *Cooper log instability is absent*, and superconductivity arises from an *increase in the pairing interaction* as the temperature is lowered and the *development of long range phase coherence*
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